

The *p*-nitrophenyl rings make dihedral angles of 9.5 (1) and 89.1 (1)° with the chelation rings, while the phenyl radicals make angles of -88.4 (1) and 14.4 (1)°.

The presence of the bulky groups in the 1 and 4 positions causes the formation of the tetrahedral complexes.

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β -Cyclodextrin–Potassium Hydroxide–Water (1/1/8)

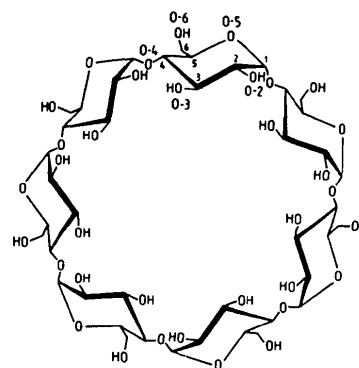
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Abstract. $C_{42}H_{70}O_{35} \cdot K^+ \cdot OH^- \cdot 8H_2O$, $M_r = 1335.24$, monoclinic, $P2_1$, $a = 15.223$ (5), $b = 10.578$ (3), $c = 20.204$ (6) Å, $\beta = 108.37$ (7)°, $V = 3087$ Å³, $Z = 2$, $D_x = 1.436$ Mg m⁻³, $\lambda(Mo K\alpha) = 0.71073$ Å, $\mu = 1.876$ mm⁻¹, $F(000) = 1420$, $T = 295$ K, final $R = 0.080$ for 4774 observed reflections. The cyclodextrin molecules are stacked, as monomeric entities, inclined at 43.4° along the twofold screw axis, forming a classical herringbone scheme. Three O atoms, attributed to water molecules, are found inside the cyclodextrin cavity, two of them being hydrogen bonded to the two primary hydroxyl groups which are in a *gauche-trans* conformation. Six others, present as doublets or singlets of water molecules, are located between the cyclodextrin entities and ensure the packing *via* hydrogen bonding. The potassium ion is incorporated in an interstitial site and coordinated to six non-water O atoms which belong to four different cyclodextrin units, in a distorted trigonal-prism environment. It is suggested that the balancing negative charge is localized inside the cavity, one of the three water molecules being in fact a hydroxyl anion.

Introduction. Cyclodextrins, cyclic oligosaccharides consisting of six, seven or eight α -1 \rightarrow 4-linked glucose units, have attracted interest owing to their ability to form inclusion compounds with a wide variety of 'guest' molecules; such complexes are used in the pharmaceutical and food industries. (Sztetli, 1989). However, their interaction with metals has



β -Cyclodextrin

received less attention; in view of the interest in cation-saccharide interactions, we have undertaken research in this field, leading to the isolation of suitable crystals of a β -cyclodextrin compound containing a potassium ion.

Experimental. The crystals were obtained from an aqueous potassium hydroxide solution of β -cyclodextrin. A colourless crystal of approximate dimensions 0.6 × 0.4 × 0.2 mm was selected, preliminarily tested by photographic methods, and then mounted on an Enraf-Nonius CAD-4 diffractometer (graphite-monochromated MoK α radiation). Cell constants from setting angles of 25 reflections in the range $8 \leq \theta \leq 12^\circ$; 8126 intensities collected at room temperature, $\omega/2\theta$ scans, $0 \leq h \leq 20$, $0 \leq k \leq 14$, $-26 \leq l \leq 26$, $2 \leq \theta \leq 28^\circ$, leading after averaging ($R_{\text{int}} = 0.034$) to 4774 reflections with $I \geq 3\sigma(I)$ used in the least-squares refinement of 573 parameters. Three standard reflections (444, 8 $\bar{4}$, 1 $\bar{2}$, 642) showed an average intensity loss of 8.6% during the data collection (112h), taken into account in a decay correction. Lorentz and polarization corrections; empirical absorption correction from φ scans (0.95–1.00).

The structure was solved starting from positional parameters of β -cyclodextrin in the related structure of the complex β -cyclodextrin-benzyl alcohol (Harata, Uekama, Otagiri, Hirayama & Ohtani, 1985). Full-matrix least-squares minimization of $\sum w(\Delta F)^2$ with $w = 1/(\sigma F)^2$ and $\sigma F = [(\sigma I)^2 + (pF)^2]^{1/2}/2F$, p being an experimental instability factor, estimated at 0.06. Only potassium (as a cation) and oxygen were given anisotropic temperature factors; H atoms bonded to C atoms introduced in ideal positions, not refined. Atomic scattering factors were from *International Tables for X-ray Crystallography* (1974, Vol. IV). All calculations were carried out with the SDP chain of programs (Frenz, 1988) on a Digital MicroVAX computer. Final agreement factors $R = 0.080$, $wR = 0.107$. $(\Delta/\sigma)_{\text{max}} = 0.10$. $(\Delta\rho)_{\text{min,max}} = -0.40, 0.38 \text{ e } \text{\AA}^{-3}$. Final atomic coordinates and equivalent isotropic thermal parameters are given in Table 1.*

Discussion. The structure reveals that the potassium ion is trapped in the lattice external to the cyclodextrin cavity.

The β -cyclodextrin molecules form, through the 2₁ axis, a herringbone-like pattern along the bc plane

Table 1. Fractional coordinates and equivalent isotropic thermal parameters for the K and O atoms with e.s.d.'s in parentheses

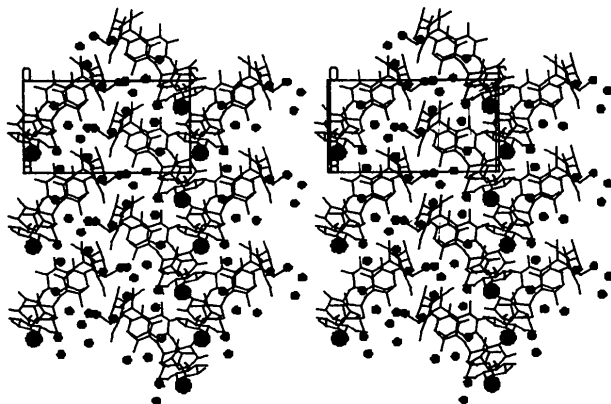
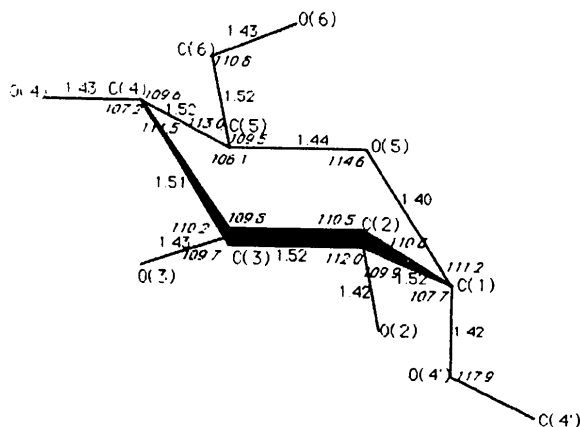
	x	y	z	$B_{\text{eq}}(\text{\AA}^2)$
K ⁺	0.4596 (2)	0.788	0.0551 (1)	4.64 (5)*
C(11)	-0.1361 (5)	0.0935 (8)	0.3680 (4)	2.9 (1)
C(21)	-0.2038 (5)	0.0466 (9)	0.2995 (4)	2.9 (1)
C(31)	-0.1959 (5)	0.1257 (8)	0.2408 (4)	2.7 (1)
C(41)	-0.2128 (5)	0.2639 (8)	0.2554 (4)	2.6 (1)
C(51)	-0.1486 (5)	0.3066 (8)	0.3271 (4)	2.8 (1)
C(61)	-0.1759 (6)	0.436 (1)	0.3486 (5)	3.8 (2)
O(21)	-0.1888 (4)	-0.0831 (7)	0.2923 (3)	3.9 (1)*
O(31)	-0.2620 (4)	0.0924 (6)	0.1764 (3)	3.5 (1)*
O(41)	-0.1962 (3)	0.3398 (6)	0.2020 (3)	2.9 (1)*
O(51)	-0.1540 (4)	0.2194 (6)	0.3804 (2)	3.0 (1)*
O(61)	-0.2693 (4)	0.4318 (7)	0.3457 (3)	4.8 (2)*
C(12)	0.2112 (5)	-0.0628 (9)	0.4707 (4)	3.0 (1)
C(22)	0.1341 (5)	-0.1565 (9)	0.4533 (4)	3.2 (2)
C(32)	0.0506 (5)	-0.1038 (9)	0.3978 (4)	3.0 (1)
C(42)	0.0255 (5)	0.0231 (8)	0.4203 (4)	2.9 (1)
C(52)	0.1069 (5)	0.1124 (9)	0.4409 (4)	3.1 (2)
C(62)	0.0855 (7)	0.235 (1)	0.4722 (6)	5.1 (2)
O(22)	0.1638 (4)	-0.2739 (7)	0.4323 (3)	4.0 (1)*
O(32)	-0.0236 (4)	-0.1922 (7)	0.3850 (3)	4.2 (1)*
O(42)	-0.0465 (3)	0.0782 (8)	0.3626 (2)	3.2 (1)*
O(52)	0.1845 (4)	0.0531 (7)	0.4921 (3)	3.7 (1)*
O(62)	0.1546 (7)	0.323 (1)	0.4807 (6)	8.8 (3)*
C(13)	0.4795 (5)	-0.0474 (8)	0.3567 (4)	2.8 (1)
C(23)	0.4271 (6)	-0.1728 (9)	0.3506 (4)	3.4 (2)
C(33)	0.3285 (5)	-0.1490 (9)	0.3507 (4)	2.9 (1)
C(43)	0.3330 (5)	-0.0731 (9)	0.4144 (4)	2.8 (1)
C(53)	0.3870 (5)	0.0477 (9)	0.4184 (4)	3.1 (1)
C(63)	0.4015 (6)	0.123 (1)	0.4859 (5)	4.1 (1)
O(23)	0.4297 (5)	-0.2389 (7)	0.2901 (3)	4.4 (1)*
O(33)	0.2803 (4)	-0.2633 (6)	0.3479 (3)	3.9 (1)*
O(43)	0.2393 (3)	-0.0439 (6)	0.4105 (3)	3.0 (1)*
O(53)	0.4791 (3)	0.0161 (6)	0.4166 (3)	3.3 (1)*
O(63)	0.4396 (5)	0.0496 (9)	0.5451 (3)	5.1 (2)*
C(14)	0.5034 (5)	0.2362 (8)	0.1463 (4)	2.7 (1)
C(24)	0.5050 (5)	0.0940 (8)	0.1378 (4)	2.7 (1)
C(34)	0.4531 (5)	0.0294 (8)	0.1827 (4)	2.9 (1)
C(44)	0.4923 (5)	0.0750 (8)	0.2571 (4)	2.7 (1)
C(54)	0.4903 (5)	0.2207 (8)	0.2602 (4)	2.6 (1)
C(64)	0.5338 (6)	0.272 (1)	0.3323 (4)	3.6 (2)
O(24)	0.4684 (4)	0.0565 (7)	0.0668 (3)	3.7 (1)*
O(34)	0.4641 (5)	-0.1048 (6)	0.1792 (3)	4.1 (1)*
O(44)	0.4350 (3)	0.0229 (6)	0.2949 (2)	2.7 (1)*
O(54)	0.5405 (3)	0.2698 (6)	0.2171 (3)	2.9 (1)*
O(64)	0.6270 (5)	0.2305 (8)	0.3632 (3)	4.9 (2)*
C(15)	0.2610 (5)	0.5839 (8)	0.0157 (4)	2.5 (1)
C(25)	0.2839 (5)	0.4842 (8)	-0.0303 (4)	2.7 (1)
C(35)	0.3205 (5)	0.3631 (8)	0.0098 (4)	2.5 (1)
C(45)	0.3963 (5)	0.3915 (8)	0.0751 (4)	2.4 (1)
C(55)	0.3716 (5)	0.4965 (9)	0.1177 (4)	2.9 (1)
C(65)	0.4547 (7)	0.544 (1)	0.1750 (5)	4.7 (2)
O(25)	0.2035 (4)	0.4639 (7)	-0.0897 (3)	3.4 (1)*
O(35)	0.3569 (4)	0.2807 (7)	-0.0317 (3)	4.2 (1)*
O(45)	0.4115 (3)	0.2765 (6)	0.1161 (4)	2.8 (1)*
O(55)	0.3393 (4)	0.6066 (6)	0.0743 (3)	3.0 (1)*
O(65)	0.5267 (5)	0.5800 (9)	0.1470 (4)	6.2 (2)*
C(16)	-0.0680 (6)	0.6842 (9)	0.0384 (5)	3.5 (2)
C(26)	-0.0586 (5)	0.6551 (9)	-0.0332 (4)	3.2 (2)
C(36)	0.0258 (5)	0.5729 (9)	-0.0265 (4)	2.8 (1)
C(46)	0.1106 (5)	0.6294 (9)	0.0270 (4)	3.0 (1)
C(56)	0.0922 (5)	0.6534 (9)	0.0954 (4)	3.1 (2)
C(66)	0.1722 (6)	0.718 (1)	0.1488 (5)	4.4 (2)
O(26)	-0.1408 (4)	0.5919 (9)	-0.0744 (3)	4.9 (2)*
O(36)	0.0413 (4)	0.5644 (8)	-0.0928 (3)	3.9 (1)*
O(46)	0.1860 (3)	0.5440 (6)	0.0369 (3)	2.8 (1)*
O(56)	0.0144 (4)	0.7360 (6)	0.0831 (3)	3.5 (1)*
O(66)	0.1567 (5)	0.7267 (9)	0.2162 (3)	5.3 (2)*
C(17)	-0.2614 (5)	0.4374 (9)	0.1730 (4)	3.0 (1)
C(27)	-0.2953 (5)	0.4178 (8)	0.0949 (4)	2.6 (1)
C(37)	-0.2162 (5)	0.4442 (9)	0.0640 (4)	2.9 (1)
C(47)	-0.1701 (5)	0.5690 (8)	0.0882 (4)	2.6 (1)
C(57)	-0.1426 (5)	0.5791 (9)	0.1676 (4)	3.3 (2)
C(67)	-0.1087 (8)	0.709 (1)	0.1946 (6)	5.6 (2)
O(27)	-0.3329 (3)	0.2945 (7)	0.0772 (3)	3.3 (1)*
O(37)	-0.2560 (4)	0.4400 (9)	-0.0109 (3)	4.8 (2)*
O(47)	-0.0907 (3)	0.5700 (6)	0.0655 (3)	3.0 (1)*
O(57)	-0.2203 (4)	0.5564 (6)	0.1907 (3)	3.5 (1)*
O(67)	-0.1905 (6)	0.7971 (8)	0.1751 (4)	7.5 (2)*
OW(2)	0.7035 (6)	0.063 (1)	0.4699 (4)	6.9 (2)*
OW(3)	0.6236 (6)	0.017 (1)	0.5752 (4)	7.1 (2)*
OW(4)	0.2853 (7)	0.332 (2)	0.6155 (6)	10.4 (4)*
OW(5)	0.3983 (6)	0.1319 (9)	0.6587 (4)	6.9 (2)*

* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and full lists of bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54052 (44 pp.). Copies may be obtained through the Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1 (cont.)

	x	y	z	$B_{\text{eq}}(\text{\AA}^2)$
OW(6)	0.0744 (7)	0.953 (1)	0.2162 (4)	7.7 (3)*
OW(7)	0.6461 (9)	0.770 (1)	0.199 (1)	15.4 (6)*
OW(8)	0.103 (1)	0.482 (2)	0.2663 (7)	13.3 (5)*
OW(9)	0.001 (1)	0.276 (2)	0.1867 (9)	18.1 (6)*
OW(10)	0.044 (1)	0.511 (1)	0.3867 (9)	14.1 (5)*

$$* B_{\text{eq}} = (4/3) \sum_i \sum_j \beta_{ij} a_i \cdot a_j.$$


 Fig. 1. Packing view of the structure down the a axis showing the herringbone scheme.

 Fig. 2. Average bond distances (\AA) and angles ($^\circ$) for the seven glucose units.

(Fig. 1) as monomer units; other members of this monomeric class differ essentially in the nature of the included molecules inside the cavity: water molecules (Lindner & Saenger, 1982a; Betzel, Saenger, Hingerty & Brown, 1984; Zabel, Saenger & Mason, 1986); ethanol (Tokuoka, Abe, Fujiwara, Tomita & Saenger, 1980); methanol and HI (Lindner & Saenger, 1982b); nicotinamide (Harata, Kawano, Fukunaga & Ohtani, 1983); hexamethylenetetramine (Harata, 1984); benzyl alcohol (Harata *et al.*, 1985). In all these structures, external water molecules ensure the packing *via* hydrogen bonds.

Table 2. Torsion angles around the C5—C6 bonds and tilt angles

Glucose unit	Torsion angles ($^\circ$)		Tilt angles ($^\circ$)
	C(4)—C(5)—C(6)—O(6)	O(5)—C(5)—C(6)—O(6)	
1	54.9 (9)	-65.8 (8)	-3.9 (1.6)
2	-170.5 (9)	68.0 (1.0)	23.1 (6)
3	52.8 (1.0)	-66.5 (9)	11.4 (1.1)
4	56.2 (1.0)	-63.7 (9)	10.6 (6)
5	53.3 (1.1)	-65.4 (1.0)	15.0 (6)
6	-173.6 (8)	66.8 (1.0)	26.6 (6)
7	71.1 (1.0)	-49.6 (9)	10.7 (9)

Tilt angles are defined as the angles between the O4 plane and the C(1)—C(4)—O(4)—O(4') planes.

In the potassium- β -cyclodextrin compound the average bond distances and angles are in the correct range for the seven glucose residues (Fig. 2). The O(4) plane of the β -cyclodextrin molecule is inclined at 43.4° on the ac plane. The distances (\AA) to the least-squares plane are in order from O(41) to O(47): 0.285(6), 0.031(6), $-0.293(6)$, 0.078(5), 0.298(6), $-0.0269(5)$ and $-0.130(6)\text{\AA}$. The distances O($4n$)—O($4n + 1$) range from 4.327(7) to 4.436(8) \AA and the radius of the heptagon (distance from the centre of gravity) is between 4.93 and 5.20 \AA , showing no critical differences for any elliptical distortion.

The torsion angles concerning the orientation of the C(6)—O(6) bonds show two different types of conformation, *gauche-trans* for G2 and G6 and *gauche-gauche* for the other residues (Table 2).

The mean O(6) plane is parallel to the O(4) plane although the O(6) atoms which are in *gauche-trans* conformations are most distant from the plane (0.8 \AA).

Strong intermolecular hydrogen bonding is seen either between hydroxyl groups themselves or between water molecules and hydroxyl groups (Table 3). In contrast to other structures of this type, no disorder was found, neither in water nor primary hydroxyl positions. However, the internal water molecules are affected by higher thermal motion than the six external ones, of which only OW(7) has an elongated thermal ellipsoid.

There exists intermolecular primary hydroxyl bonding, 2.74 \AA , between O(61) and O(64) ensuring strong cohesion along the a axis, which is also reinforced by the bonding through OW(7) between O(65) and O(67) (both distances 2.69 \AA) in the same direction. Two very short intermolecular distances, 2.59 and 2.43 \AA , are observed between, respectively, two secondary hydroxyl groups, O(25) and O(31), symmetry related ($-x, \frac{1}{2} + y, -z$), and between the same hydroxyl O(25) and a primary hydroxyl O(67), symmetry related ($-x, -\frac{1}{2} + y, -z$). These contribute to the formation of a cyclodextrin double layer structure, parallel to the ab plane and alternatively centred at the $z = 0$ and $z = \frac{1}{2}$ levels.

The role played by the primary hydroxyl groups in the cohesion of the structure is essential, in that sense

Table 3. Possible schemes for hydrogen bonding about the O atoms of the water molecules, and primary and secondary hydroxyl groups

Distances in Å and angles in °.

Water molecules	Atom 1	Atom 2		
OW(2)	OW(3)	OW(4)	3.03	114
	OW(3)	O(64)	2.75	121.9
	O(22)	O(64)	-	100.6
	OW(4)	O(64)	-	99.2
OW(3)	OW(2)	O(63)	2.69	118.4
	O(33)	O(63)	-	109.2
OW(4)	OW(2)	O(21)	2.86	104.4
	OW(5)	O(21)	-	116.3
	OW(5)	O(62)	2.82	118.2
	O(21)	O(62)	-	106.7
OW(5)	OW(4)	O(61)	2.87	102.2
	OW(4)	O(63)	2.71	105.8
	OW(4)	O(23)	2.84	99.3
OW(6)	O(66)	O(36)	2.82	122.1
OW(7)	O(21)	O(34)	2.98	113.8
	O(65)	O(67)	2.69	124.1
OW(8)	OW(9)	OW(10)	2.87	107.5
	OW(10)	O(66)	2.99	112.9
OW(9)	OW(8)	O(41)	3.19	98.2
	O(36)	O(41)	-	101.9
OW(10)	OW(8)	O(62)	2.89	102.1
	O(22)	O(62)	-	96.6
Primary hydroxyls				
O(61)	OW(5)	O(64)	2.74	99.3
O(63)	OW(3)	OW(5)	2.71	110.7
O(64)	OW(2)	O(61)	2.74	118.9
O(66)	OW(6)	O(33)	2.73	98.2
	OW(8)	O(56)	2.87	98.1
O(67)	OW(7)	O(25)	2.43	109.2
	O(21)	O(25)	-	105.1
	O(21)	O(57)	2.62	107.9
Secondary hydroxyls				
O(25)	O(31)	O(36)	2.67	106.8
	O(35)	O(46)	2.78	97.3
O(31)	O(25)	O(41)	2.79	115.1
	O(21)	O(41)	-	115.1
O(32)	O(22)	O(42)	2.90	114.2
O(33)	O(43)	O(66)	2.73	106.8
	O(43)	O(23)	2.88	115.2
O(34)	OW(7)	O(24)	2.86	96.7
	OW(7)	O(44)	2.85	118.7
	O(24)	O(44)	-	114.7
O(35)	O(25)	O(45)	2.84	111.0
O(36)	OW(9)	O(25)	2.67	109.9
	O(26)	O(46)	2.85	112.3
O(37)	O(27)	O(47)	2.86	112.7

they fix a 'cortège' of water molecules, either as doublets, OW(2)—OW(3), respectively by O(64) and O(63), OW(4)—OW(5), respectively by O(62) and O(63), or singlets OW(6) by O(66), OW(7) by O(65) and O(67), at an average distance of 2.73 Å, always shorter than the distances water—secondary hydroxyl group (average 2.89 Å), see Fig. 3.

The particular orientation of the C(6)—O(6) bonds of the G2 and G6 residues probably results from hydrogen bonding of the primary hydroxyls O(62) and O(66) with internal water molecules OW(8) and OW(10). The third internal 'water' molecule OW(9) is clearly located deeper within the cavity. While OW(8) and OW(10) straddle the mean O6 plane (+0.66 and -0.87 Å, respectively), OW(9) is close to the O4 plane (+0.48 Å) and displaced from the O4 centroid towards O(41). Although at a distance of 2.86 Å from OW(8),

OW(9) is best hydrogen bonded between O(41) and O(36) with an angle of 101.9°. The bonding to O36 (2.87 Å) is of interest, as this atom belongs to the symmetry related $(-x, -\frac{1}{2} + y, -z)$ cyclodextrin unit: the bonding then traverses the cavity (or *trans*-cavity). This observation led us to suspect that OW(9) acts as a counterion of the K^+ cation present outside the cavity, in the form of a hydroxyl anion. It has been seen in some α -cyclodextrin ionic complexes that anions are generally located inside the cavity, while cations prefer interstitial sites (McMullan, Saenger, Fayos & Mootz, 1973). The K^+ site corresponds to a position generally occupied by a water molecule in the related monomeric structures.

The environment of the potassium ion is comprised of six O atoms (four secondary hydroxyls, one primary hydroxyl, one ring atom and no water oxygen) in a highly distorted trigonal prism, as shown in Fig. 4, but none of the six O atoms seems

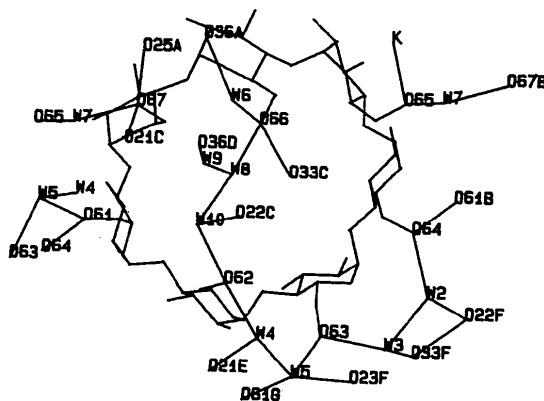


Fig. 3. The β -cyclodextrin molecular unit with water molecules and significant interacting atoms from adjacent cyclodextrin molecules. Symmetry code: $A -x, \frac{1}{2} + y, -z$; $B 1 + x, y, z$; $C x, 1 + y, z$; $D -x, -\frac{1}{2} + y, -z$; $E -x, \frac{1}{2} + y, 1 - z$; $F 1 - x, \frac{1}{2} + y, 1 - z$; $G -x, -\frac{1}{2} + y, 1 - z$.

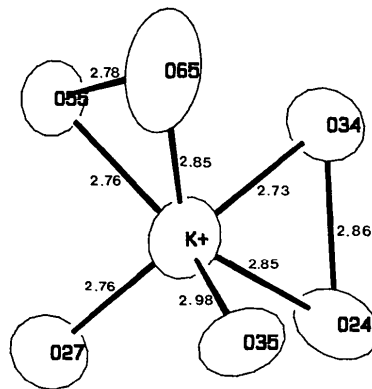


Fig. 4. The potassium environment. Distances in Å.

to play a particular role or appears to be affected by a bond of the ionic type. The distances are longer than the sum of the ionic radii of K and O (2.66 Å). Owing to coordination to the potassium ion, the local environment is modified with respect to that found about the water molecule occupying this site in other monomeric structures. Four different cyclodextrin molecules participate in the coordination, two O atoms belong to one cyclodextrin unit translated along the *b* axis [O(24) and O(34)]; two others belong to symmetry-related cyclodextrin units ($-x, \frac{1}{2} + y, -z$) [O(27) and $(1 - x, \frac{1}{2} + y, -z)$ O(35)]. The potassium ions trapped in the cyclodextrin double layers form an infinite zigzag chain with an angle of 123° along the *b* axis (Fig. 1), the K—K distance being 6.02 Å.

This structure confirms the versatility of the basic monomer β -cyclodextrin hydrate structure which here is shown capable of accepting a potassium ion without significant changes in the lattice; this is also the case for a range of hydrate structures and simple monosubstituted β -cyclodextrin derivatives now under investigation.

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Structure of 1,1,1,2,2,2-Hexacarbonyl- $\{\mu$ -3-[1(η^6)-2-methylphenyl]-2(η^4)-1-oxo-1-phenyl-2-propene}-chromiumiron

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Abstract. $[\text{CrFe}(\text{CO})_6(\text{C}_{16}\text{H}_{14})]$, $M_r = 498.19$, triclinic, $P\bar{1}$, $a = 9.719$ (1), $b = 11.143$ (2), $c = 11.860$ (3) Å, $\alpha = 100.76$ (15), $\beta = 113.7$ (16), $\gamma = 107.98$ (15)°, $V = 1045$ Å³, $Z = 2$, $D_x = 1.58$ g cm⁻³, $\lambda(\text{Mo } K\alpha) = 0.71069$ Å, $\mu = 11.4$ cm⁻¹, $T = 293$ K, $F(000) = 504$, $R = 0.027$ for 3361 reflections with F_o^2

$\geq 3\sigma(F_o^2)$. The relative configuration of the title complex obtained by reaction of 1-phenyl-3-(η^6 -*o*-methylphenyl)tricarbonylchromiumprop-2-en-1-one with nonacarbonyldiiron is unambiguously (*RS*, *SR*).

Introduction. Selective reactions of chiral *ortho*-substituted arene–chromium–tricarbonyl complexes have been reported (Davies & Goodfellow, 1989;

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